

Development of the AMUSE Code

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Advanced Nuclear Fuel Cycle Initiative
Quarterly Review
January 2003
Albuquerque, NM



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Purpose of AMUSE

AFCI



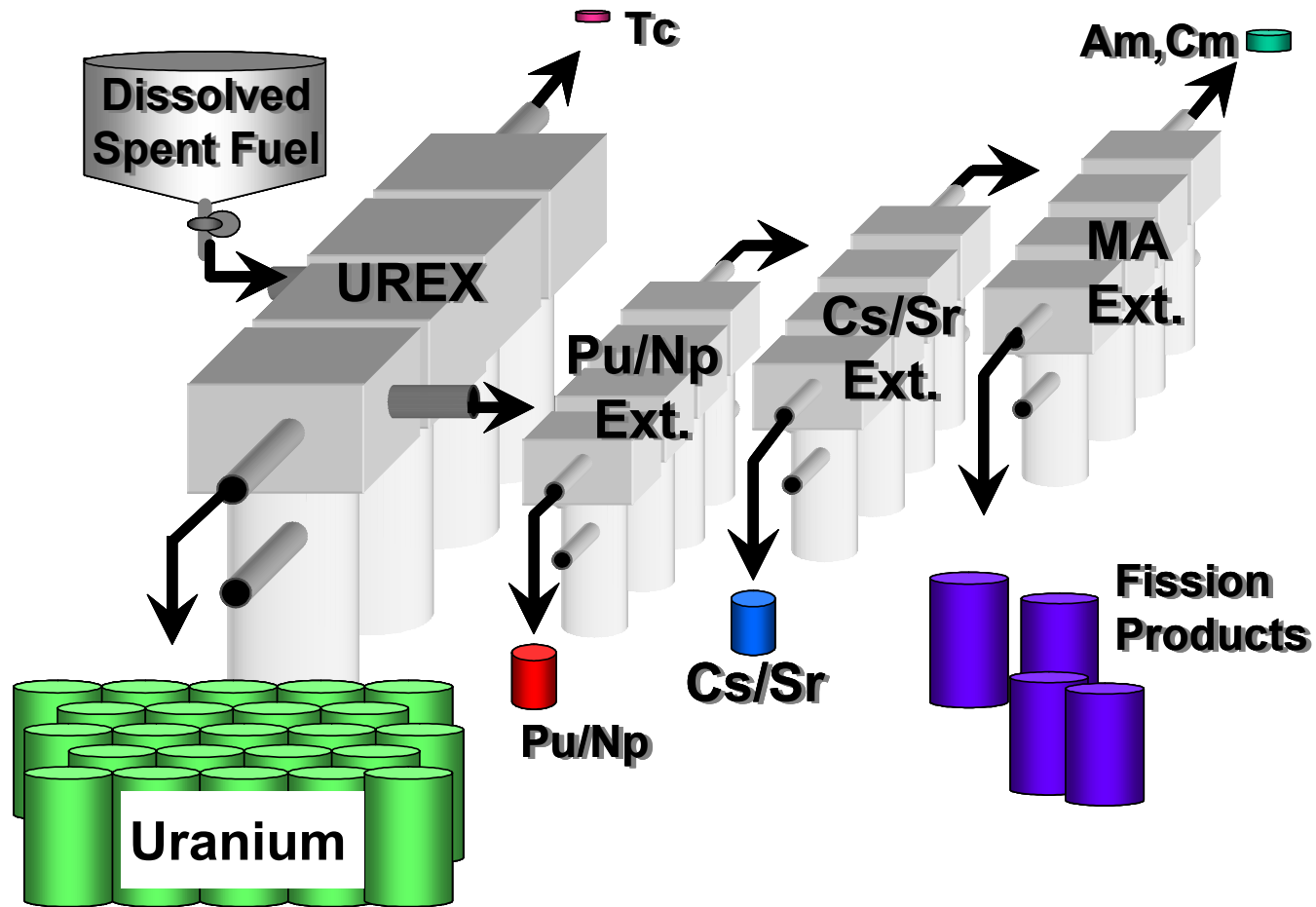
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- The UREX+ process is being developed as part of the Advanced Aqueous Process Separations
- ANL work is centered on process design, modeling, and demonstration
- **The AMUSE code forms the computational basis for flowsheet design and process development**

Advanced Aqueous Process Development – UREX+



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2003 Milestones



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- Demonstrate UREX+ with spent fuel at ANL
 - Process includes U, Tc, Pu/Np, Cs/Sr, and Am/Cm separations
- Update Model
 - Add Pu/Np, Cs/Sr, and Am/Cm extraction processes to AMUSE
- Design, with other participants, flowsheet for UREX+ engineering scale demonstration at INEEL

UREX Flowsheets Design

- AMUSE was used to design countercurrent uranium solvent-extraction process demonstrations using
 - Simulated feed in FY 01 at ANL
 - Dissolved commercial fuel in FY 02 at SRTC



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Development of AMUSE



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Basis of AMUSE

- The Generic TRUEX Model (GTM) was developed in the 1980s to calculate flowsheets for treating High-Level Liquid Waste
- The keys to its success were
 - Developing algorithms from a firm understanding of the chemistry
 - Basing D values on chemically significant equilibria
 - i.e., not just fitting experimental data to power series
 - Using thermodynamic activities for hydrogen ion, nitrate, and water to fit experimental data to equilibrium equations
 - Building the model in a modular format with the easily programmed and user-friendly Microsoft Excel



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The AMUSE Code

- The GTM was expanded to include UREX and PUREX processes
 - It is reborn as the
Argonne **M**odel for **U**niversal **S**olvent **E**xtraction (**AMUSE**)
- New front end was added for easier input
 - Currently using Visual Basic for Excel
 - Graphical user interface being developed in partnership with UNLV

AMUSE Capabilities



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- Models for Solvent Extraction
 - TRUEX, SREX, UREX and PUREX
- Applications
 - Design flowsheet to meet specific process goals
 - Optimize flowsheet for robust performance
 - Variation in feed compositions
 - Variation in feed flow rates
 - Measure effects of process deviations caused by operational upsets or product diversion



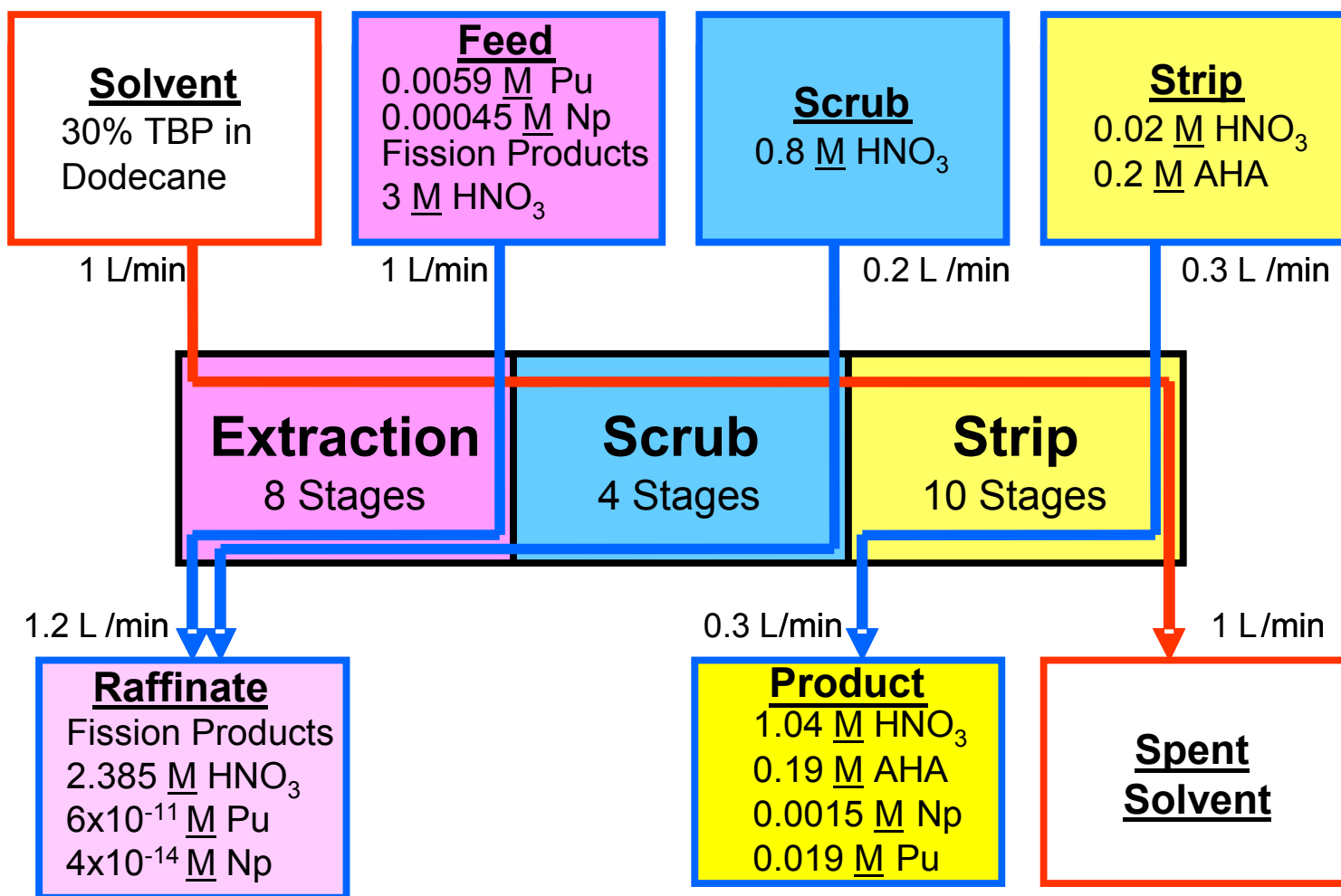
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AMUSE Simulation



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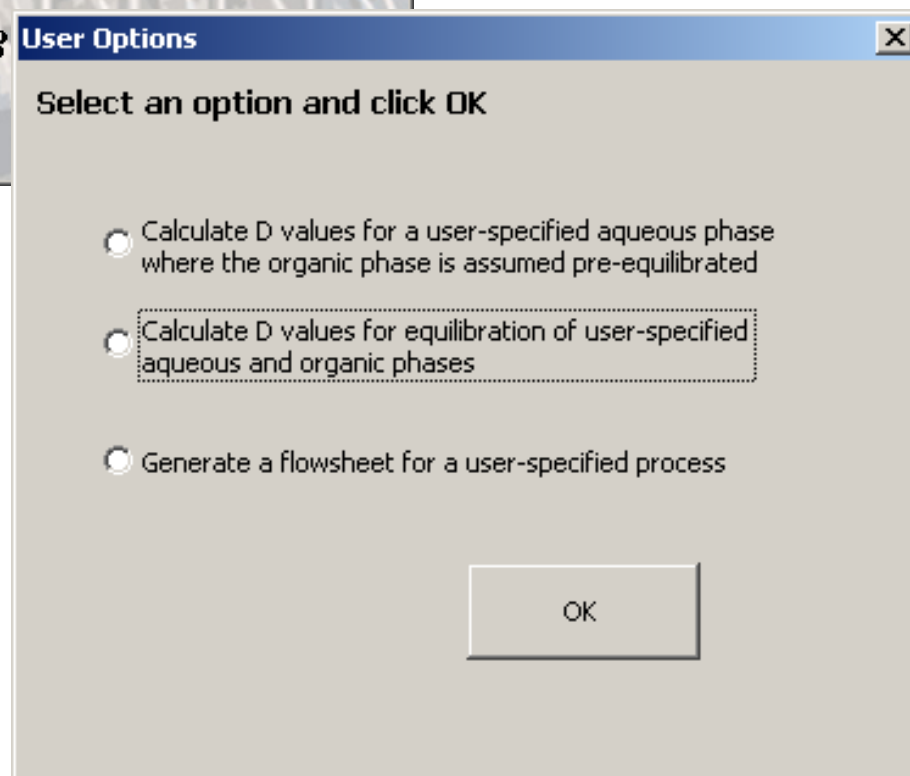
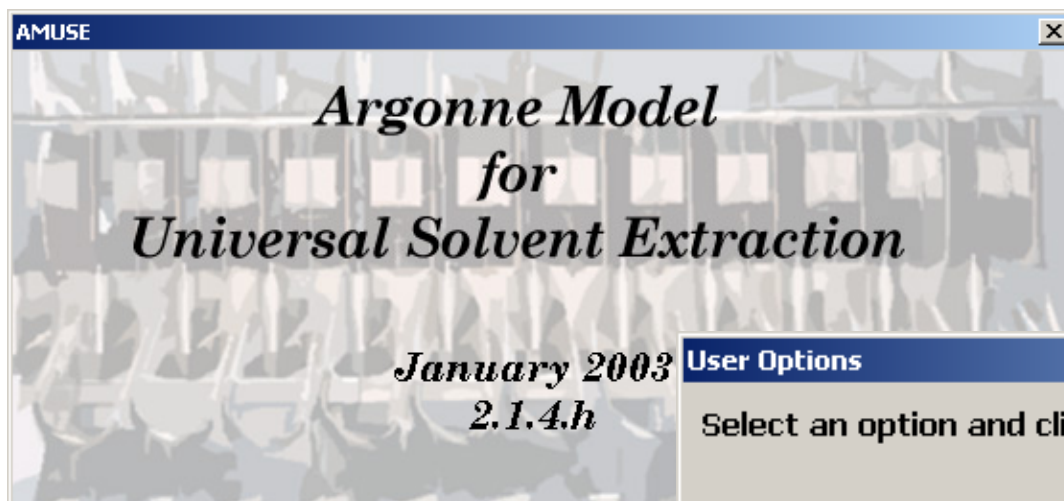
Pu/Np Separation from Fission Products



AMUSE Start-up



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General Input Form



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Update Print Run AMUSE
Verify Input Save Quit

General | Stream Identity | Section 1 | Section 2 | Section 3 | Flowsheet Display

User-specified file name: NPPEX
Directory (folder) name: reports
Number of sections: 3
Process Temperature: 25

Solvent Extraction Type
☒ Contactor
☐ Pulsed Column
☐ Mixer Settler

TBP Concentration: 1.1

Type of solvent:
☐ UREX
☒ PUREX
☐ TRUEX-NPH
☐ TRUEX-TCE
☐ TRUEX-SREX
☐ TRUEX-DAAP-SREX

Recycle Org
☐ Yes
☒ No

Flowsheet Display

```
graph TD
    Solvent --> Extraction
    Feed --> Extraction
    Scrub --> Scrub
    Strip --> Strip
    Extraction --> Raffinate
    Scrub --> Product
    Strip --> SpentSolvent[Spent Solvent]
```

The flowsheet diagram shows four input streams at the top: Solvent, Feed, Scrub, and Strip. Below them are three colored process blocks: Extraction (pink), Scrub (blue), and Strip (yellow). Arrows indicate the flow from each input stream to its corresponding process block. The Extraction block has an output arrow pointing to a Raffinate box. The Scrub block has an output arrow pointing to a Product box. The Strip block has an output arrow pointing to a Spent Solvent box.

Section Data -- Extraction



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Update Print Add Section Remove Section Run AMUSE Save Quit

General Stream Identity Section 1 Section 2 Section 3 Flowsheet Display

Section Name: Extraction Aqueous Flow Rate: 1 Organic Flow Rate: 1

Number of Stages: 8 Fraction Aq Effluent: 1 Fraction Org Effluent:

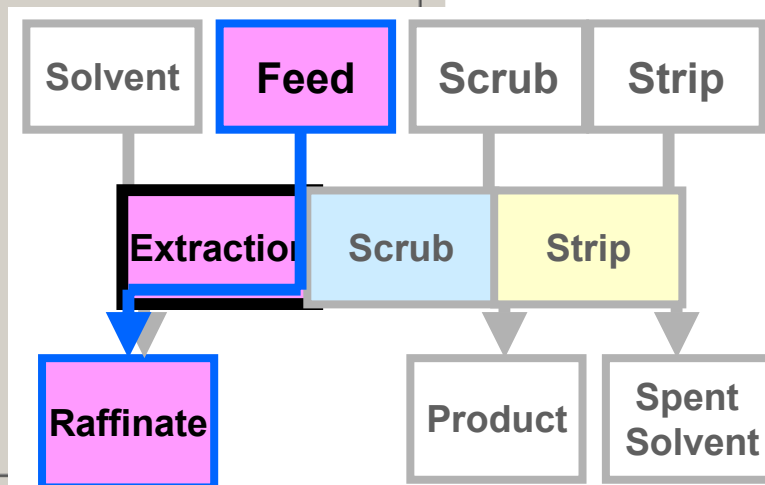
Fractional Efficiency: Aq Reroute Section: Org Reroute Section:

Fraction of Aq Entrained in the Org: 0.005 Fraction of Org Entrained in the Aq: 0.005

Aqueous Feed Organic Feed Stage Sampling Stage-Specific Input

Non-Fission-Product Cations		Fission-Products		Anions	
H (+)	3	ZrO (2+)		NO3 (-)	3.02405
Fe (3+)		Rb (+)		F (-)	
Cr (2+)		Cd (2+)		SO4 (2-)	
Bi (3+)		Cs (+)		C2O4 (2-)	
Al (3+)		Sr (2+)		PO4 (3-)	
Na (+)		Y (3+)		TcO4 (-)	
Ca (2+)		Ba (2+)		Cl (-)	
Cu (2+)		Rh (3+)		ClO4 (-)	
Mg (2+)		Pd (2+)			
Hg (2+)		Ag (+)			
		RuNO (3+)			
Fission-Product Rare Earths		Actinides			
La (3+)		Th (4+)			
Ce (3+)		UO2 (2+)			
Pr (3+)		Np (4+)			
Nd (3+)		NpO2 (+)	.00045		
Pm (3+)		NpO2 (2+)			
Sm (3+)		Pu (3+)			
Eu (3+)		Pu (4+)	.0059		
Gd (3+)		Am (3+)			
		Cm (3+)			

Aqueous
Feed



Section Data -- Extraction



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Update Print Add Section Run AMUSE
Verify Input Remove Section Save Quit

General Stream Identity Section 1 Section 2 Section 3 Flowsheet Display

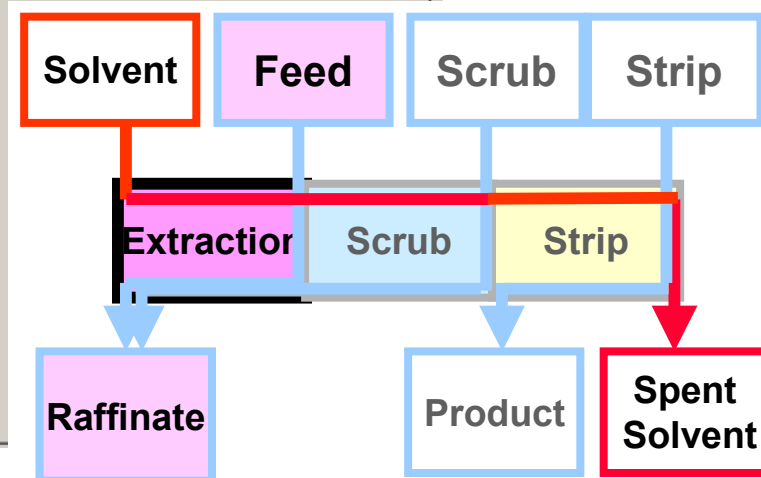
Section Name: Extraction Aqueous Flow Rate: 1 Organic Flow Rate: 1
 Number of Stages: 8 Fraction Aq Effluent: 1 Fraction Org Effluent:
 Fractional Efficiency: Aq Reroute Section: Org Reroute Section:
 Fraction of Aq Entrained in the Org: 0.005 Fraction of Org Entrained in the Aq: 0.005

Aqueous Feed Organic Feed Stage Sampling Stage-Specific Input

Non-Fission-Product Cations		Fission-Products		Anions	
H (+)		Zr (4+)		NO3 (-)	
Fe (3+)		Rb (+)		F (-)	
Cr (2+)		Cd (2+)		SO4 (2-)	
Bi (3+)		Cs (+)		C2O4 (2-)	
Al (3+)		Sr (2+)		PO4 (3-)	
Na (+)		Y (3+)		TcO4 (-)	
Ca (2+)		Ba (2+)		Cl (-)	
Cu (2+)		Rh (3+)		ClO4 (-)	
Mg (2+)		Pd (2+)			
Hg (2+)		Ag (+)			
		RuNO (3+)			

Fission-Product Rare Earths		Actinides	
La (3+)		Th (4+)	
Ce (3+)		UO2 (2+)	
Pr (3+)		Np (4+)	
Nd (3+)		NpO2 (+)	
Pm (3+)		NpO2 (2+)	
Sm (3+)		Pu (3+)	
Eu (3+)		Pu (4+)	
Gd (3+)		Am (3+)	
		Cm (3+)	

Organic
Feed



Section Data -- Scrub



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Update Print Add Section Run AMUSE
Verify Input Remove Section Save Quit

General Stream Identity Section 1 Section 2 Section 3 Flowsheet Display

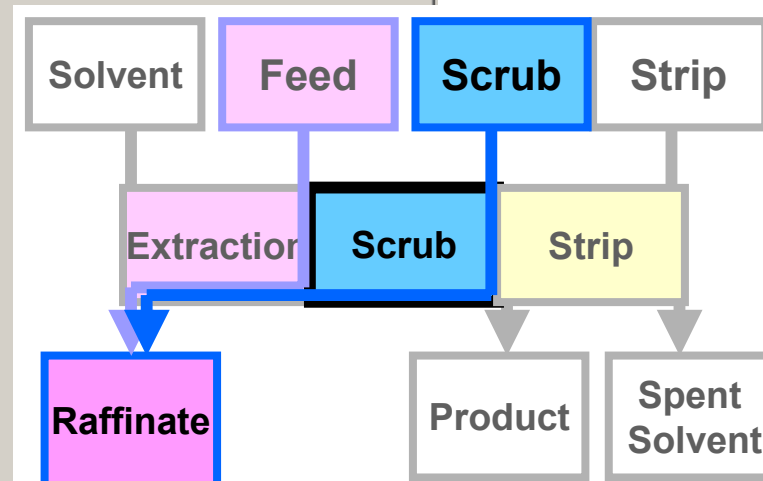
Section Name: Scrub Aqueous Flow Rate: .2 Organic Flow Rate:
 Number of Stages: 4 Fraction Aq Effluent: Fraction Org Effluent:
 Fractional Efficiency: Aq Reroute Section: Org Reroute Section:
 Fraction of Aq Entrained in the Org: 0.005 Fraction of Org Entrained in the Aq: 0.005

Aqueous Feed Organic Feed Stage Sampling Stage-Specific Input

Non-Fission-Product Cations		Fission-Products		Anions	
H (+)	.8	ZrO (2+)		NO3 (-)	0.8
Fe (3+)		Rb (+)		F (-)	
Cr (2+)		Cd (2+)		SO4 (2-)	
Bi (3+)		Cs (+)		C2O4 (2-)	
Al (3+)		Sr (2+)		PO4 (3-)	
Na (+)		Y (3+)		TcO4 (-)	
Ca (2+)		Ba (2+)		Cl (-)	
Cu (2+)		Rh (3+)		ClO4 (-)	
Mg (2+)		Pd (2+)			
Hg (2+)		Ag (+)			
		RuNO (3+)			

Fission-Product Rare Earths		Actinides	
La (3+)		Th (4+)	
Ce (3+)		UO2 (2+)	
Pr (3+)		Np (4+)	
Nd (3+)		NpO2 (+)	
Pm (3+)		NpO2 (2+)	
Sm (3+)		Pu (3+)	
Eu (3+)		Pu (4+)	
Gd (3+)		Am (3+)	
		Cm (3+)	

Aqueous
Feed

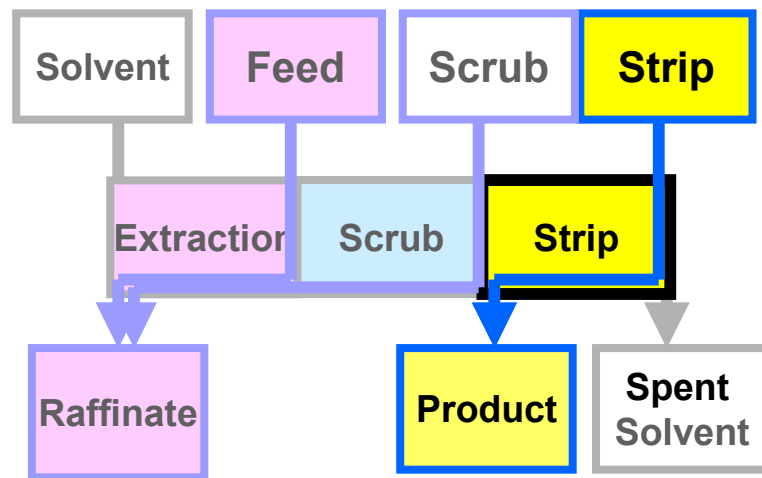


Section Data -- Strip



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Aqueous
Feed



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Update Print Add Section Run AMUSE
Verify Input Remove Section Save Quit

General Stream Identity Section 1 Section 2 Section 3 Flowsheet Display

Section Name: Strip Aqueous Flow Rate: .3 Organic Flow Rate:
Number of Stages: 10 Fraction Aq Effluent: 1 Fraction Org Effluent: 1
Fractional Efficiency: Aq Reroute Section: Org Reroute Section:
Fraction of Aq Entrained in the Org: 0.005 Fraction of Org Entrained in the Aq: 0.005

Aqueous Feed Organic Feed Stage Sampling Stage-Specific Input

Non-Fission-Product Cations		Fission-Products		Anions	
H (+)	.02	ZrO (2+)		NO3 (-)	0.02
Fe (3+)		Rb (+)		F (-)	
Cr (2+)		Cd (2+)		SO4 (2-)	
Bi (3+)		Cs (+)		C2O4 (2-)	
Al (3+)		Sr (2+)		PO4 (3-)	
Na (+)		Y (3+)		TcO4 (-)	
Ca (2+)		Ba (2+)		Cl (-)	
Cu (2+)		Rh (3+)		ClO4 (-)	
		Pd (2+)			
		Ag (+)			
		RuNO (3+)			
		Actinides		Neutral Species	
		Th (4+)		B(OH)3	
		UO2 (2+)		AHA	.2
		Np (4+)			
		NpO2 (+)			
		NpO2 (2+)			
		Pu (3+)			
		Pu (4+)			
		Am (3+)			
		Cm (3+)			

Enter all concentrations in molar units.

Stage-Specific Input



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Update Print Add Section Run AMUSE
Verify Input Remove Section Save Quit

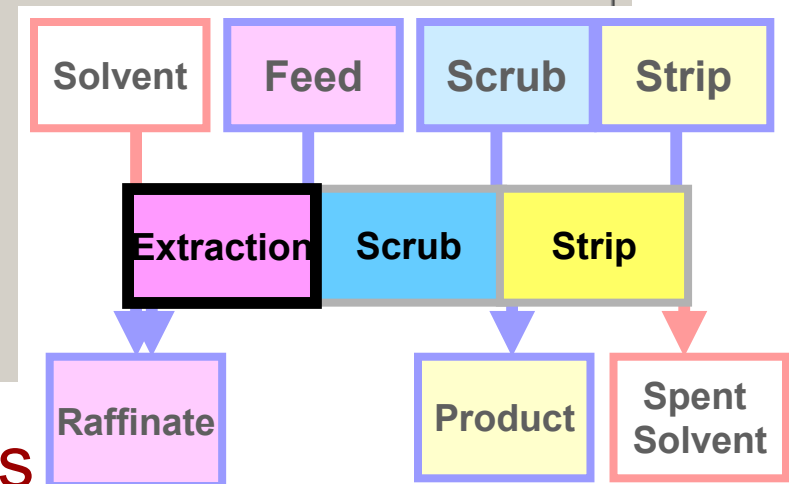
General Stream Identity Section 1 Section 2 Section 3 Flowsheet Display

Section Name: Extraction Aqueous Flow Rate: 1 Organic Flow Rate: 1
 Number of Stages: 8 Fraction Aq Effluent: 1 Fraction Org Effluent:
 Fractional Efficiency: Aq Reroute Section: Org Reroute Section:
 Fraction of Aq Entrained in the Org: 0.005 Fraction of Org Entrained in the Aq: 0.005

Aqueous Feed Organic Feed Stage Sampling Stage-Specific Input

Stage Number	Process Temperature	Fractional Efficiency
1	25	1
2	25	1
3	25	1
4	25	1
5	25	1
6	25	1
7	25	1
8	25	1

Extraction Section Stages



AMUSE Reports

GRAPHICAL

- A figure is created for each component
 - Showing its concentrations in both the organic and aqueous phase of every stage

TABULAR

- Tabular reports are created for
 - Influent and effluent compositions and flow rates
 - Stage profiles that include
 - Distribution ratios
 - Component concentrations in organic and aqueous phases

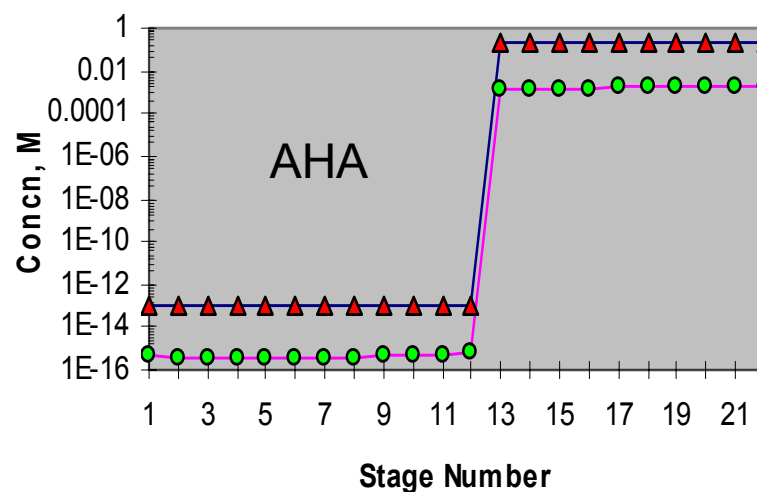
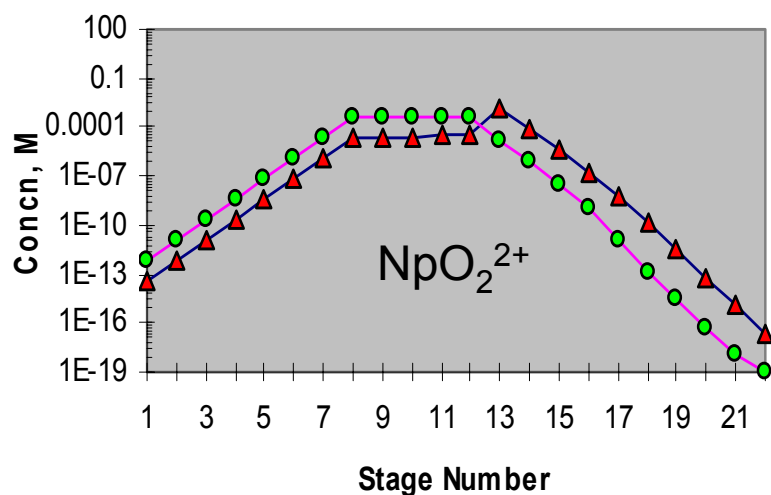
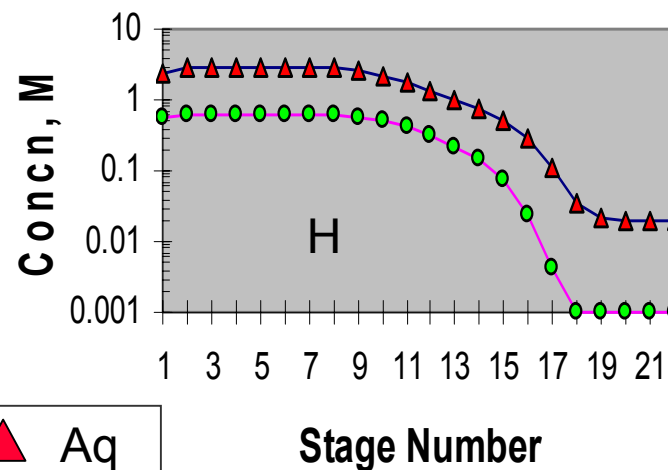
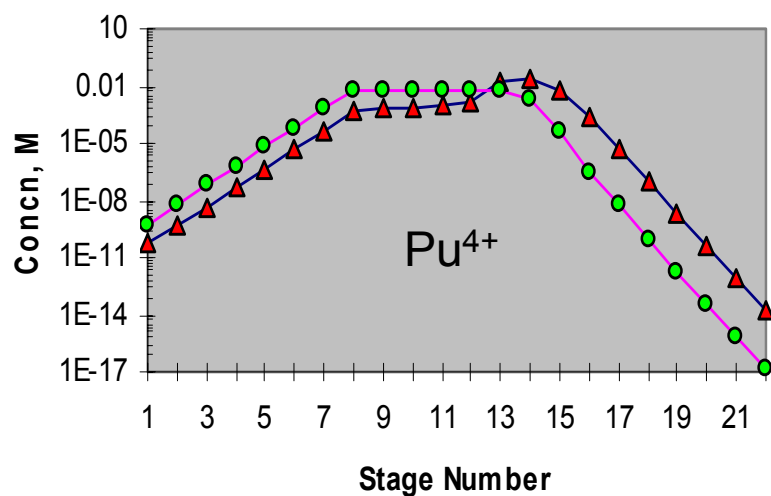


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Graphical Output



Tabular Output

Section	Name	Stage Number	Phase	Flow Direction	Stream Identity	Flow Rate	Component Concentration, M			
							H	AHA	NpO2_2	Pu_4
1	Extraction	1	O	in	DX	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	Extraction	8	A	in	DF	1	3.000E+00	1.000E-13	4.500E-04	5.900E-03
2	scrub	12	A	in	DS	0.2	8.000E-01	1.000E-13	0.000E+00	0.000E+00
3	strip	22	A	in	EF	0.3	2.000E-02	2.000E-01	0.000E+00	0.000E+00
1	Extraction	1	A	out	DW	1.1949749	2.385E+00	9.952E-14	3.829E-14	5.980E-11
3	strip	13	A	out	EW	0.3050266	1.035E+00	1.915E-01	1.475E-03	1.934E-02
3	strip	22	O	out	EP	1	1.926E-04	1.594E-03	2.196E-20	1.506E-17



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Component Name Phase			Stage-to-Stage Profile for each Component			
			Section No. Stage No. 1	1 2	1 3	1 4
H	Aqueous	x, M	2.385E+00	2.836E+00	2.912E+00	2.923E+00
		y, M	5.416E-01	6.296E-01	6.435E-01	6.457E-01
		D value	2.271E-01	2.220E-01	2.210E-01	2.209E-01
AHA	Aqueous	x, M	9.952E-14	9.989E-14	9.986E-14	9.985E-14
		y, M	4.387E-16	4.020E-16	3.964E-16	3.955E-16
		D value	4.408E-03	4.024E-03	3.969E-03	3.961E-03
NpO2_2	Aqueous	x, M	3.829E-14	5.675E-13	9.857E-12	1.769E-10
		y, M	7.100E-13	1.313E-11	2.365E-10	4.269E-09
		D value	1.854E+01	2.313E+01	2.399E+01	2.413E+01
Pu_4	Aqueous	x, M	5.980E-11	4.870E-10	4.704E-09	4.702E-08
		y, M	5.450E-10	5.895E-09	5.959E-08	5.998E-07
		D value	9.114E+00	1.210E+01	1.267E+01	1.276E+01

3 20	3 21	3 22
2.011E-02	2.001E-02	2.000E-02
1.945E-04	1.927E-04	1.926E-04
9.675E-03	9.632E-03	9.629E-03
2.000E-01	2.000E-01	2.000E-01
1.594E-03	1.594E-03	1.594E-03
7.968E-03	7.968E-03	7.968E-03
5.630E-14	1.114E-15	2.196E-17
5.630E-17	1.114E-18	2.196E-20
1.000E-03	1.000E-03	1.000E-03
3.862E-11	7.639E-13	1.506E-14
3.862E-14	7.639E-16	1.506E-17
1.000E-03	1.000E-03	1.000E-03



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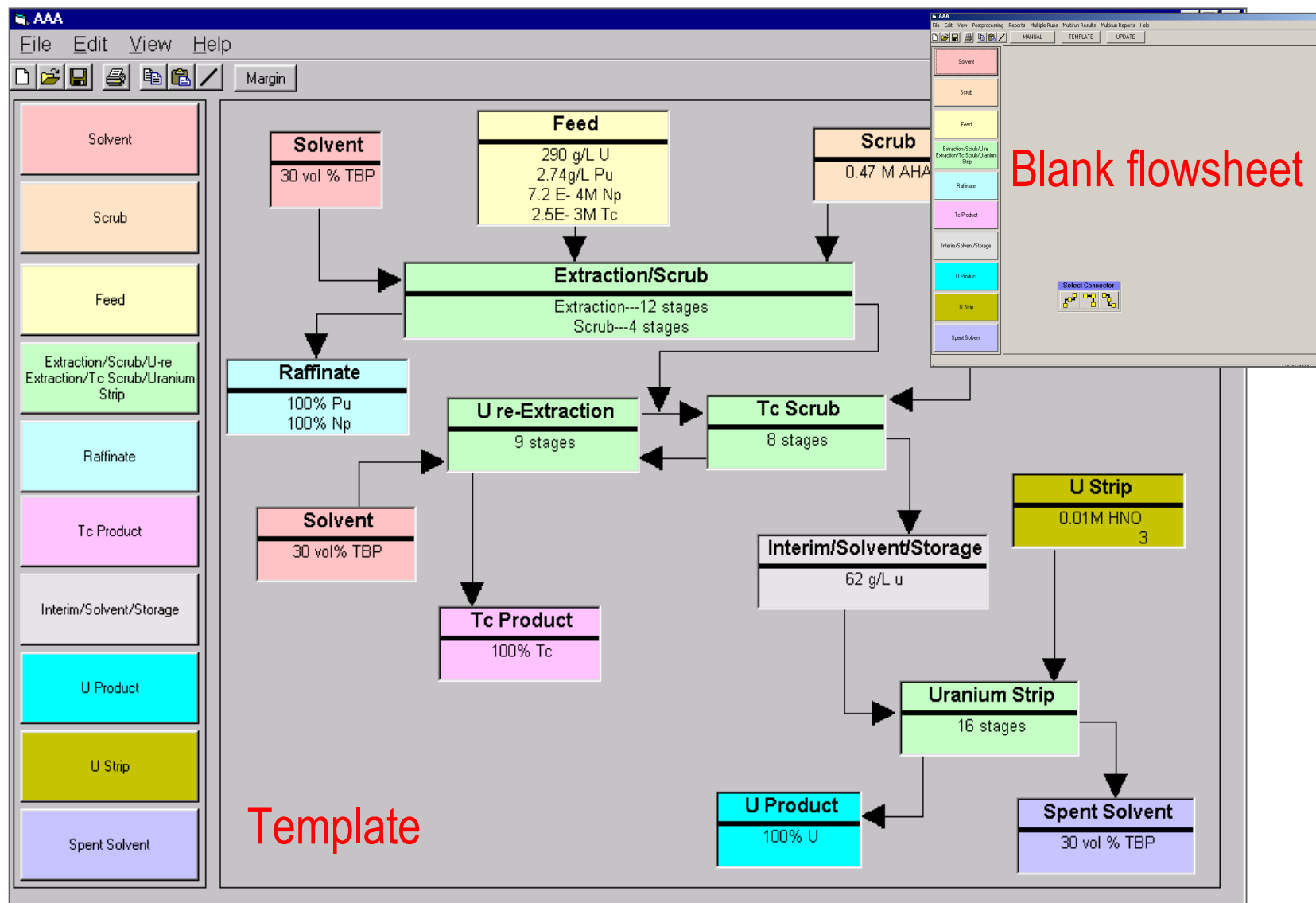
UNLV Partnership

- Working with Nevada Center for Advanced Computational Methods (NCACM)
 - Developing and implementing a graphical user interface (GUI) for AMUSE
 - Designing a systems-engineering model to optimize the UREX+ process

Graphical User Interface



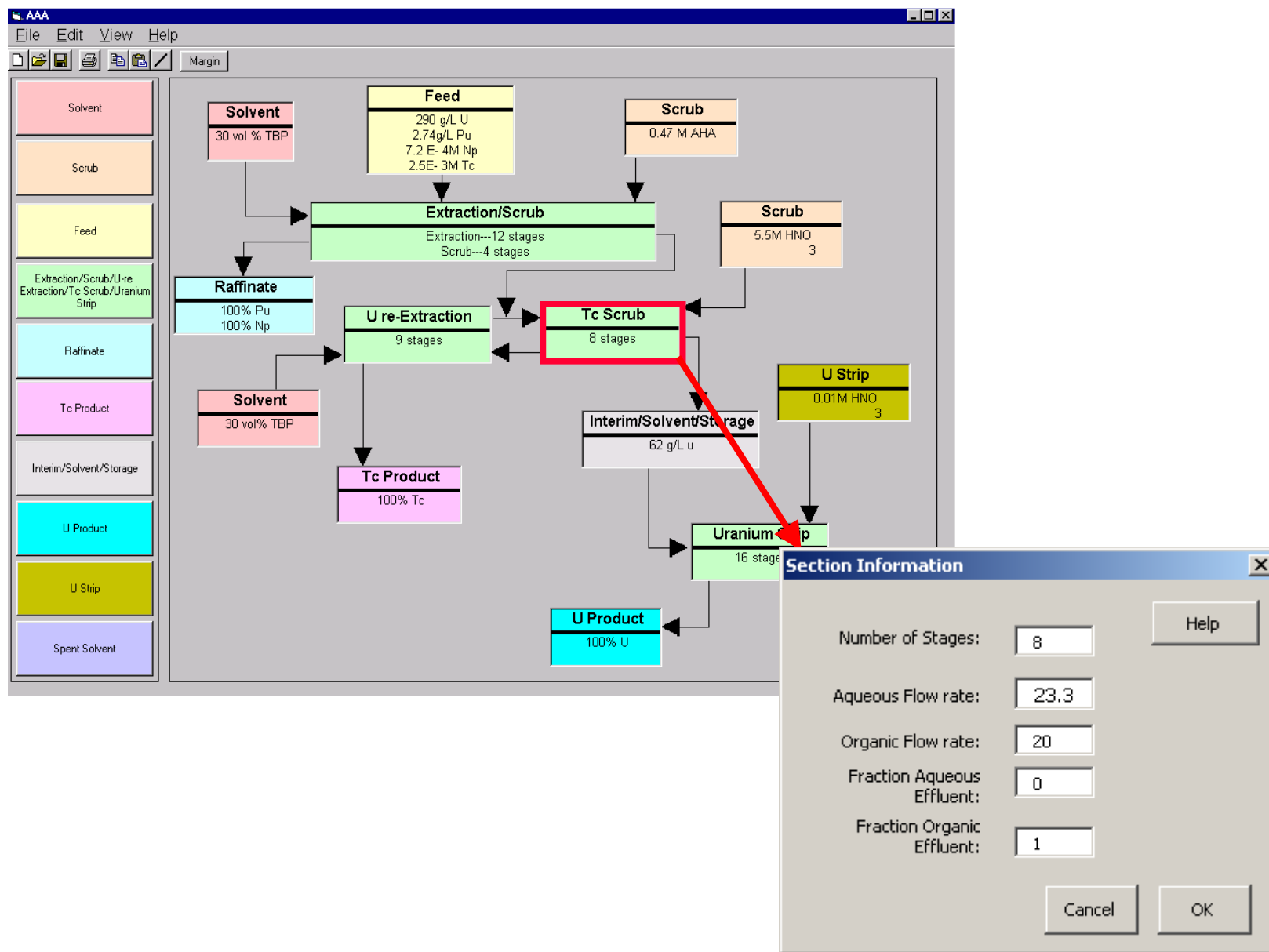
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Graphical User Interface



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Participants from NCACM

- Faculty
 - Dr. Yitung Chen - Principal Investigator
 - Dr. Randy Clarksean - Co-Principal Investigator
 - Dr. Hsuan-Tsung (Sean) Hsieh – Interface and database design and development
- Graduate Students
 - Lijian Sun – Systems engineering model design
 - Haritha Royyuru – Interface design and implementation



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Conclusion and Future Development

Conclusion

- AMUSE has been an important tool for developing the UREX process and will continue to be for the UREX+ process



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Future Model Development

- Add all potential UREX+ processes
 - Using literature data
 - Data collected at SRTC, ORNL, INEEL, LANL and ANL
- Improve model predictions based on
 - Demonstration results
 - Fundamental studies in collaboration with MIT
- Develop monitor-and-control parameters for UREX+ process